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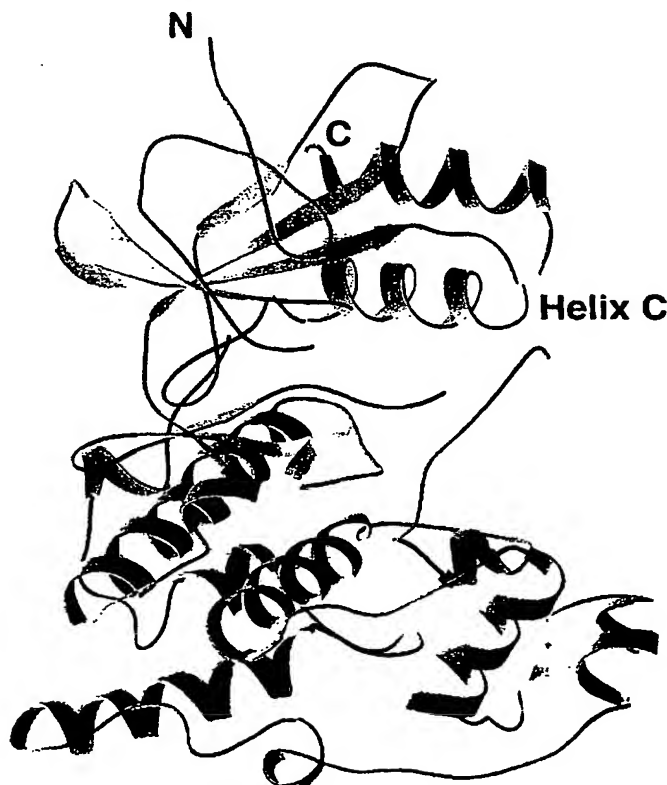
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[Continued on next page]

(54) Title: CRYSTAL STRUCTURES OF JNK-INHIBITOR COMPLEXES AND BINDING POCKETS THEREOF



(57) Abstract: The invention relates to crystalline molecules or molecular complexes that comprise binding pockets of c-Jun N-terminal kinase 3 (JNK3) or its homologues. The invention also relates to crystals comprising JNK3 and an inhibitor. The present invention also relates to a computer comprising a data storage medium encoded with the structural coordinates of JNK3 binding pockets and methods of using a computer to evaluate the ability of a compound to bind to the molecule or molecular complex. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for, design and optimize compounds, including agonists and antagonists, which bind to JNK3 or homologues thereof.

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**Declarations under Rule 4.17:**

- *as to applicant's entitlement to apply for and be granted a patent (Rule 4.17(ii)) for the following designations* AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, *ARIPO patent* (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), *Eurasian patent* (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), *European patent* (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR), *OAPI patent* (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG)
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